

6-Benzyl-6,7-dihydro-5H-pyrrolo[3,4-B]pyridine
109966-30-5 | DTXSID50364043

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 6.80

Global applicability domain: Inside

Local applicability domain index: 4.98e-01

Confidence level: 5.58e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>4-Isobutylmorpholine</div> <div>Measured: 1.78</div> <div>Predicted: 2.69</div>	<div>Image not found</div> <div>N,N-Dimethyl-1,2-dithiolan-4-amine</div> <div>Measured: 52.5</div> <div>Predicted: 17.5</div>	<div>Image not found</div> <div>Thiram</div> <div>Measured: 3.39</div> <div>Predicted: 3.91</div>
<div>Image not found</div> <div>Molinate</div> <div>Measured: 25.7</div> <div>Predicted: 14.8</div>	<div>Image not found</div> <div>Isophorone</div> <div>Measured: 2.00</div> <div>Predicted: 3.19</div>	